

i's

(FILE 'HOME' ENTERED AT 09:53:11 ON 16 DEC 2004)

FILE 'REGISTRY' ENTERED AT 09:53:26 ON 16 DEC 2004

L1 1 S MALPHOS/CN
L2 0 S DUPHOS/CN
L3 0 S DUPHOS/CN

FILE 'CAPLUS' ENTERED AT 09:54:31 ON 16 DEC 2004

L4 5 S L1

FILE 'REGISTRY' ENTERED AT 09:59:21 ON 16 DEC 2004

L5 STR
L6 1 S L5

FILE 'CAPLUS' ENTERED AT 10:03:28 ON 16 DEC 2004

L7 1 S L6
S L5

FILE 'REGISTRY' ENTERED AT 10:03:45 ON 16 DEC 2004

L8 1 S L5

FILE 'CAPLUS' ENTERED AT 10:03:45 ON 16 DEC 2004

L9 1 S L8

FILE 'REGISTRY' ENTERED AT 10:04:18 ON 16 DEC 2004

L10 30 S L5 FUL

FILE 'CAPLUS' ENTERED AT 10:04:38 ON 16 DEC 2004

L11 149 S L10

FILE 'REGISTRY' ENTERED AT 10:05:26 ON 16 DEC 2004

L12 STR L5
L13 15 SEARCH L12 SUB=L10 FUL

FILE 'CAPLUS' ENTERED AT 10:08:48 ON 16 DEC 2004

L14 137 S L13
L15 102 S L13/CAT
L16 90 S ME-DUPHOS
L17 171 S L15 OR L16
L18 0 S 11 27 123 126 135 CBIB ABS

FILE 'REGISTRY' ENTERED AT 10:21:16 ON 16 DEC 2004

L19 STR
L20 0 S L19
L21 2 S L19 FUL

FILE 'CAPLUS' ENTERED AT 10:24:58 ON 16 DEC 2004

L22 237 S L 21
L23 5 S L21
L24 0 S L21 NOT L4

=> fil reg

FILE 'REGISTRY' ENTERED AT 10:26:26 ON 16 DEC 2004

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Property values tagged with IC are from the ZIC/VINITI data file
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STRUCTURE FILE UPDATES: 14 DEC 2004 HIGHEST RN 797749-23-6

DICTIONARY FILE UPDATES: 14 DEC 2004 HIGHEST RN 797749-23-6

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

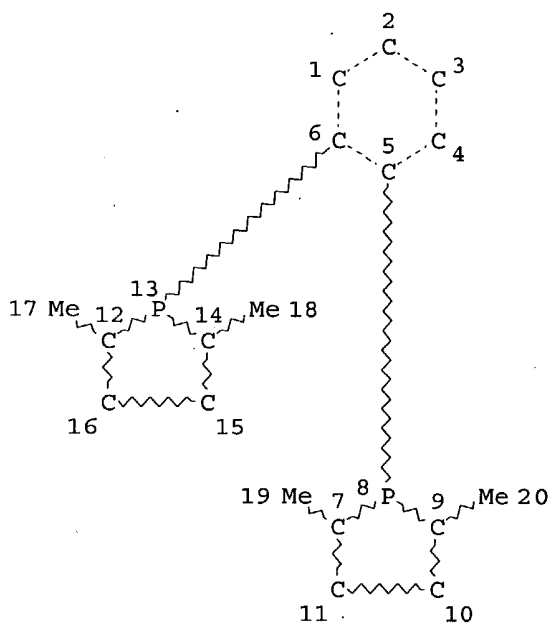
*** YOU HAVE NEW MAIL ***

'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> d l5 sia

L5 HAS NO ANSWERS

L5 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

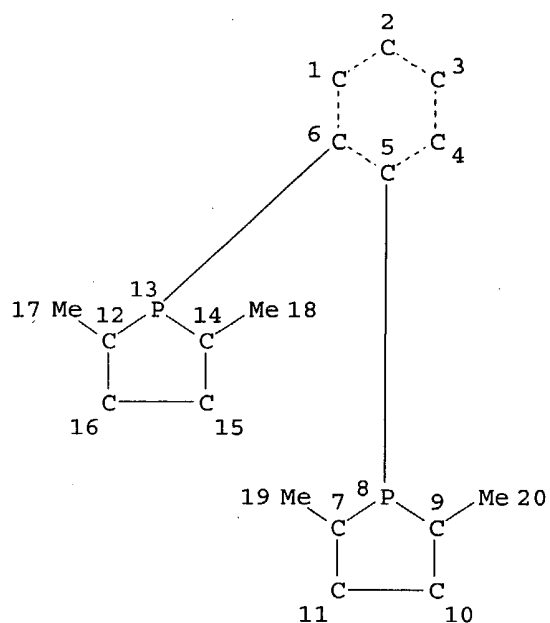
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

=> d l12 sia

L12 HAS NO ANSWERS

L12 STR



NODE ATTRIBUTES:

CONNECT IS E2 RC AT 1
 CONNECT IS E2 RC AT 2
 CONNECT IS E2 RC AT 3
 CONNECT IS E2 RC AT 4
 CONNECT IS E3 RC AT 7
 CONNECT IS E3 RC AT 9
 CONNECT IS E2 RC AT 10
 CONNECT IS E2 RC AT 11
 CONNECT IS E3 RC AT 12
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 CONNECT IS E2 RC AT 15
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 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

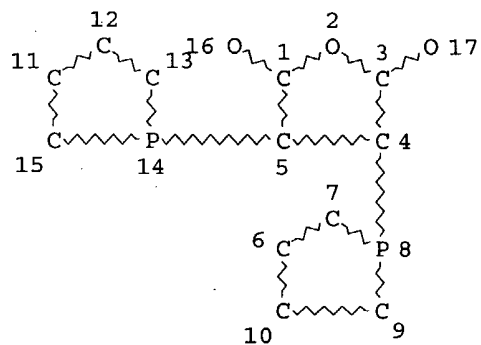
STEREO ATTRIBUTES: NONE

=>

=> d l19 sia

L19 HAS NO ANSWERS

L19 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

*** YOU HAVE NEW MAIL ***

'REGISTRY' IS DEFAULT FORMAT FOR 'REGISTRY' FILE

=> s malphos/cn

L1 1 MALPHOS/CN

=> s duphos/cn

L2 0 DUPHOS/CN

=> s DuPhos/cn

L3 0 DUPHOS/CN

=> fil caplus

FILE 'CAPLUS' ENTERED AT 09:54:31 ON 16 DEC 2004

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FILE COVERS 1907 - 16 Dec 2004 VOL 141 ISS 25

FILE LAST UPDATED: 15 Dec 2004 (20041215/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l1

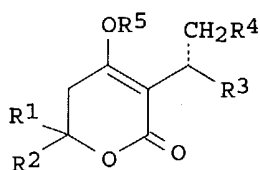
L4 5 L1

=> d tot chib abs

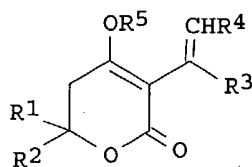
L4 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

2004:822753 Document No. 141:332050 Enantioselective hydrogenation of intermediates for the synthesis of tipranavir. Klingler, Franz; Steigerwald, Michael; Ehlenz, Richard (Boehringer Ingelheim Pharma G.m.b.H. & Co. K.-G., Germany). Ger. Offen. DE 10313118 A1 20041007, 10 pp. (German). CODEN: GWXXBX. APPLICATION: DE 2003-10313118 20030324.

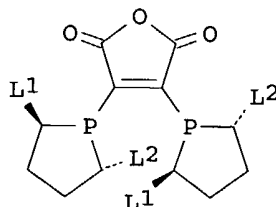
GI



I



II



III

AB The invention concerns a procedure for the production of the compds. I [R1, R2 = H, C1-6-alkyl, C3-8-cycloalkyl, C6-10-aryl, (C1-4-alkylene)-(C6-10-aryl) {optionally substituted 1 - 3 times with OH, NH2, NHCOMe, N(COMe)2, halogen, CF3, C1-4-alkoxy}, with the proviso that R1 ≠ R2; R3 = meta-substituted Ph (substituents selected from F, Cl, Br, I, OH, O3SCF3, NO2, NH2, NHSO2-{4-(trifluoromethyl)pyridin-2-yl}, N(CH2-aryl)2), NY1Y2; Y1, Y2 = H, CO2-alkyl, CO2CH2-aryl, CO-alkyl, CO-aryl; R4 = H, C1-8-alkyl; R5 = H, SiMe3, Li, Na, K, Cs, N(R')4; R' = C1-8-alkyl, CH2-aryl] by enantioselective hydrogenation of the compds. II in presence of special hydrogenation catalysts containing the bisphospholane ligands III [L1, L2 = (un)branched C1-8-alkyl]. The invention is characterized by a high enantioselectivity, whereby the simple entrance to a substance class important drug, i.e. to intermediates of the tipranavir synthesis becomes possible. Thus, I [R1 = α-PH(CH2)2, R2 = β-Pr, R3 = C6H4NO2-3, R4 = Me, R5 = H] was hydrogeanted in MeOH containing Na2CO3 and catalytic Malphos[Rh+(COD)] BF4- to give 80% II with a purity of 98%.

L4 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
2004:570037 Document No. 141:123759 Catalytic asymmetric reductive amination of ketones via transition metal complex catalysts with chiral phosphine ligands. Zhang, Xumu (Penn State Research Foundation, USA). PCT Int. Appl. WO 2004058982 A2 20040715, 22 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-US34955 20031105. PRIORITY: US 2002-PV424663 20021106.

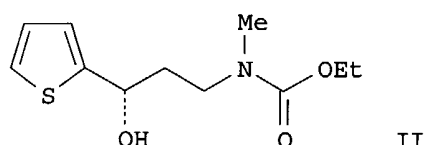
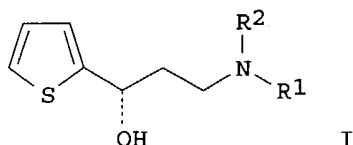
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Processes for the preparation of compds., e. g. I, having a chiral carbon substituted with an amine are disclosed. The processes include admixing a ketone, e. g. II, with an amine, e. g. III in the presence of a catalyst having a chiral phosphine ligand, e. g. IV, and an acid. The admixt. can also contain a reducing additive. The admixt. is then exposed to hydrogen to directly and asym. aminate the ketone.

L4 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
2004:101154 Document No. 140:163699 Process for the preparation of 3-hydroxy-(2-thienyl)propanamines by catalytic enantioselective hydrogenation of the corresponding ketones. Hems, William; Rossen, Kai; Reichert, Dietmar; Koehler, Klaus; Almendra Perea, Juan Jose (Degussa A.-G., Germany). PCT Int. Appl. WO 2004011452 A1 20040205, 27 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-EP7927 20030721. PRIORITY: DE 2002-10233724 20020724; DE 2002-10258098 20021211.

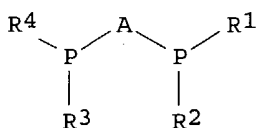
GI



AB Title compds. I [wherein R1 and R2 = independently H, (cyclo)alkyl, acyl, alkoxy carbonyl, (hetero)aryl, (hetero)aralkyl, alkylcycloalkyl, alkyl(hetero)aryl; or NR1R2 = (un)substituted heterocyclyl], intermediates for the synthesis of enantiomer-pure bioactive substances, were prepared by catalytic enantioselective hydrogenation of the corresponding α -heteroaryl ketones. Inter alia Ru catalysts with chiral diamine and chiral biphosphine ligands were used. For example, 3-[N-ethoxycarbonyl-N-methylamino]-1-(2-thienyl)-1-propanone was introduced to a Buchi stirred autoclave, which was then evacuated. A mixture of (R)-TolBINAP-RuCl₂-(1R,2R)-diphenylethylenediamine and KOBu-t in iPrOH was added. Flushing with H₂, pressurizing to 10 bar, and heating to 40° for 2 h provided II in >96% yield with an enantiomeric excess of 80.1%. The content of cyclic carbamate byproduct increased significantly after standing for a fairly long time.

L4 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
 2003:818434 Document No. 139:307895 Preparation of bisphosphines as bidentate ligands and their use as cocatalysts for asymmetric reactions. Boerner, Armin; Holz, Jens; Monsees, Axel; Riermeier, Thomas; Kadyrov, Renat; Schneider, Carsten A.; Dingerdissen, Uwe; Drauz, Karlheinz (Degussa A.-G., Germany). PCT Int. Appl. WO 2003084971 A1 20031016, 45 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2003-EP2162 20030303. PRIORITY: DE 2002-10214988 20020404.

GI



AB The present invention relates to the preparation of ligands, I (R1-R4 = independent of each other C1-8 alkyl, C2-8 alkoxyalkyl, C6-18 aryl, C7-19 aralkyl, C3-18 heteroaryl, C4-19 heteroaralkyl, C1-8-alkyl-C6-18-aryl, C1-8-alkyl-C3-18-heteroaryl, C3-8-cycloalkyl, C1-8-alkyl-C3-8-cycloalkyl, C3-8-cycloalkyl-C1-8-alkyl; R1-R2, and/or R3-R4 = C3-5 alkylene bridge mono or polysubstituted with C1-8 alkyl, HO-(C1-8)-alkyl, (C1-8)-alkoxy, (C2-8)-alkoxyalkyl, (C6-18)-aryl, etc.; A = (un)substituted heterocyclic structure), useful as cocatalysts with transition metal catalyzed asym. reactions, is described. Thus, reaction of 2,3-dichloromaleic anhydride with (R,R)-2,5-dimethyl-1-trimethylsilylphospholane (preparation given) gave 2,3-bis[(R,R)-2,5-dimethyl-phospholanyl]maleic anhydride which on treatment with [Rh(COD)₂]BF₄ in THF gave the catalyst which was used for asym. hydrogenation of unsatd. substrates, e.g. Me acetamidocinnamate.

L4 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

2003:114261 Document No. 138:287918 Synthesis of a New Chiral Bisphospholane Ligand for the Rh(I)-Catalyzed Enantioselective Hydrogenation of Isomeric β -Acylamido Acrylates. Holz, Jens; Monsees, Axel; Jiao, Haijun; You, Jinsong; Komarov, Igor V.; Fischer, Christine; Drauz, Karlheinz; Borner, Armin (Institut fuer Organische Katalyseforschung, Universitaet Rostock e.V., Rostock, 18055, Germany). Journal of Organic Chemistry, 68(5), 1701-1707 (English) 2003. CODEN: JOCEAH. ISSN: 0022-3263. OTHER SOURCES: CASREACT 138:287918. Publisher: American Chemical Society.

AB The highly stereoselective synthesis of a chiral silylphospholane has been described, which can be advantageously used as a building block under base-free conditions for the construction of diphosphines related to DuPHOS. The utility of silylphospholane is shown in the synthesis of a new bisphospholane ligand (MalPHOS), which is characterized by a maleic anhydride backbone. The ligand forms with Rh(I) a complex with a larger bite angle P-Rh-P than the analog Me-DuPHOS complex. Both complexes have been tested in the asym. hydrogenation of unsatd. α - and β -amino acid precursors of pharmaceutical relevance. In several cases, the new catalyst was superior in comparison to the Me-DuPHOS complex, in particular when (Z)-configured β -acylamido acrylates were used as substrates.

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